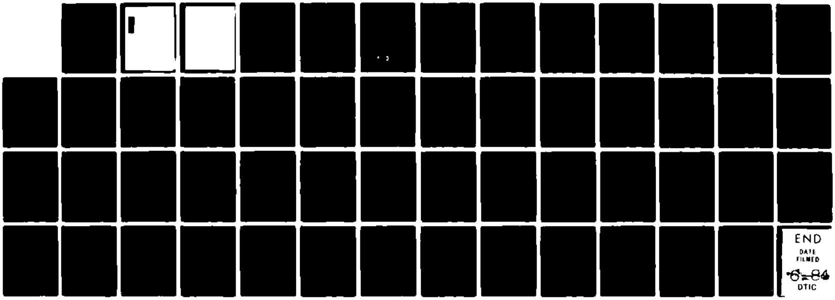
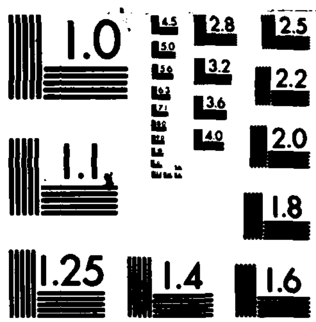
AD-A140 766 EVALUATION TECHNIQUES FOR CE-QUAL-R1: A ONE-DIMENSIONAL 1/1
RESERVOIR WATER Q..(U) ARMY ENGINEER WATERWAYS
EXPERIMENT STATION VICKSBURG MS ENVIR.. J H WLOSINSKI
UNCLASSIFIED JAN 84 WES/MP/E-84-1 F/G 13/2 NL





MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS-1963-A

AD-A140 766

Unclassified

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER Miscellaneous Paper E-84-1	2. GOVT ACCESSION NO. AD-A140 766	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) EVALUATION TECHNIQUES FOR CE-QUAL-R1: A ONE-DIMENSIONAL RESERVOIR WATER QUALITY MODEL		5. TYPE OF REPORT & PERIOD COVERED Final report
		6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) Joseph H. Wlosinski		8. CONTRACT OR GRANT NUMBER(s)
9. PERFORMING ORGANIZATION NAME AND ADDRESS U. S. Army Engineer Waterways Experiment Station Environmental Laboratory P. O. Box 631, Vicksburg, Miss. 39180		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS EWQOS Work Unit IC.1
11. CONTROLLING OFFICE NAME AND ADDRESS Office, Chief of Engineers, U. S. Army Washington, D. C. 20314		12. REPORT DATE January 1984
		13. NUMBER OF PAGES 49
14. MONITORING AGENCY NAME & ADDRESS(if different from Controlling Office)		15. SECURITY CLASS. (of this report) Unclassified
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited.

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

Available from National Technical Information Service, 5285 Port Royal Road, Springfield, Va. 22151

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

CE-QUAL-R1 (Computer program) (LC)
Computer programs (LC)
Mathematical models (LC)
Reservoirs (LC)
Water quality (LC)

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

A one-dimensional reservoir water quality model, CE-QUAL-R1, is currently being developed for use by U. S. Army Corps of Engineers District and Division Offices. Tests are needed which will ensure that model predictions are satisfactory. Although the literature contains much information concerning model evaluation, there is little agreement among authors concerning specific tests.

Two general types of tests are proposed. The first group of tests are used to ensure that the coding of the model is correct, and the (Continued)

DD FORM 1 JAN 73 1473 EDITION OF 1 NOV 65 IS OBSOLETE

Unclassified

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

20. ABSTRACT (Continued).

second group to ensure that the model predictions are suitable for the needs of the Corps. The latter tests include both qualitative and quantitative comparisons of model predictions with field-measured values. It is argued here that a thorough model evaluation must include comparisons of fluxes between variables, as well as comparisons of the mass or concentrations of variables.

PREFACE

This report is sponsored by the Office, Chief of Engineers, U. S. Army, OCE, as part of the Environmental Water Quality and Operational Studies (EWQOS) Work Unit IC.1, entitled Improve and Verify Existing One-Dimensional Reservoir Water Quality and Ecological Predictive Techniques. The OCE Technical Monitors for EWQOS were Mr. Earl Eiker, Mr. John Bushman, and Mr. James L. Gottesman.

Work for this report was conducted during the period October 1981-March 1982 by Dr. Joseph H. Wlosinski, Water Quality Modeling Group (WQMG) of the Environmental Laboratory (EL). The draft report was reviewed by Drs. Carol Collins and Allan S. Lessem, Mr. Jack B. Waide, and Ms. Linda S. Johnson.

The study was conducted under the direct supervision of Mr. Aaron Stein, Acting Chief, WQMG, and Mr. D. L. Robey, Chief, Ecosystem Research and Simulation Division, and under the general supervision of Dr. John Harrison, Chief, EL, U. S. Army Engineer Waterways Experiment Station (WES). Program Manager of EWQOS was Dr. J. L. Mahloch, EL.

Director of WES during this study and the preparation of this report was COL Tilford C. Creel, CE. Technical Director was Mr. F. R. Brown.

This report should be cited as follows:

Wlosinski, J. H. 1984. "Evaluation Techniques for CE-QUAL-R1: A One-Dimensional Reservoir Water Quality Model," Miscellaneous Paper E-84-1, U. S. Army Engineer Waterways Experiment Station, Vicksburg, Miss.

CONTENTS

EVALUATION TECHNIQUES FOR CE-QUAL-R1: A ONE-DIMENSIONAL RESERVOIR WATER QUALITY MODEL

PART I: INTRODUCTION

Background

1. One of the highest priority needs of U. S. Army Corps of Engineers (CE) District and Division Offices is the ability to realistically predict and assess the effects of engineering activities on the environment (Keeley et al. 1978). To help assess engineering effects on reservoir water quality, a one-dimensional mathematical model called CE-QUAL-R1 (Environmental Laboratory 1982) which includes physical, chemical, and biological factors is being developed as part of the Environmental Water Quality and Operational Studies (EWQOS) Program. The forerunner of CE-QUAL-R1 was the reservoir portion of a model called Water Quality for River-Reservoir Systems (WQRRS), which was assembled in 1974 for the U. S. Army Engineer Hydrologic Engineering Center, Davis, California, by Water Resources Engineers, Inc. CE-QUAL-R1, which resides on the Boeing Mainstream-EKS interactive time-sharing computer system, has been used in the past to evaluate preimpoundment water quality problems and the effects of reservoir operation on water quality (see, for example, Ford et al. 1977, 1979 and Thornton et al. 1976, 1977).

2. Another task within the EWQOS Program includes long-term comprehensive reservoir field studies (Work Unit VIIA). These field studies have provided data which are especially suitable for use with CE-QUAL-R1. Data from DeGray Reservoir, Arkansas, and Eau Galle Reservoir, Wisconsin, have been used here to provide information for improving predictive capabilities for CE-QUAL-R1; these data were collected at biweekly or monthly intervals, usually at meter increments of depth, a scheme which is suitable for evaluating the model.

Purpose

3. The purpose of this report is to discuss methods to be used for evaluating the mathematical model CE-QUAL-R1. Tests are proposed to ensure that the coding of the model is correct and to ensure that model predictions are suitable for the needs of CE District and Division Offices. The proposal includes comparisons of model predictions with field-measured values. The actual utilization of these methods to evaluate the application of CE-QUAL-R1 to DeGray and Eau Galle Reservoirs will be discussed in subsequent reports.

PART II: LITERATURE REVIEW

4. Although the literature contains much information concerning model evaluation, there is little agreement among authors. In fact, most modelers cannot agree on terminology. Not only are different terms used for the same process, but the same term is used for different processes. For example, the process of comparing model output to field-measured values is referred to as validation by a number of authors (e.g., House 1974, Miller 1974, Hall and Day 1977, Schruben 1980, and Gentil and Blake 1981) but as verification by others (e.g., Orlob 1975, Weatherbe 1976, Bedford and Babajimopoulos 1980, Thomann 1980, and Reckhow 1981). In addition, verification has been used by House (1974) and Mihram (1972) to describe a means to test the consistency of model design or its intended algorithmic structure, whereas the same general process is termed validation by Lawler (1980). Goodall (1972) also used the term validation, but he suggested that the process will not tell us if a model is valid or invalid. O'Neill (1975) wrote that it is possible to invalidate or validate the same model by manipulation of the questions asked. Caswell (1976) wrote that predictive models should be validated, and theoretical models corroborated. In reviewing Caswell's paper, Wiegert (1975) accepted the term corroboration but said that acceptance might be a more preferable term than validation. Nolan (1972) verified coding and assumptions but validated hypotheses and recognition of perception filters. Mankin et al. (1977) suggested that one should dismiss the question of model validity and ask instead whether or not the model is useful.

5. Although the terminology, number of steps, and methods may not be agreed upon by authors, tests for the evaluation of models generally involve two processes. The first process tests whether or not the model responds in the manner that the modeler intended; this process involves "debugging" the model, but should include other tests as well (Mihram 1972). Mihram suggested a systematic test that determines some specific set of environmental conditions for which the model's response should be known. A similar test was suggested by Lawler (1980), who

recommended using repetitive input and boundary conditions and checking the values of the state variables after sufficient time had elapsed for the model to dampen transient behavior.

6. The second process compares model predictions with field-measured values in an attempt to demonstrate that the model acceptably simulates the real world. It is this process about which most has been written, but upon which most disagreement remains. Even though the questions "Has the model been verified?" or "Has the model been validated?" are often asked, a number of authors state that a valid model is impossible. Goodall (1972) stated that since models are simplifications, they will virtually never be exact representations of conditions in the real world. He argued that the question of whether or not a model should be accepted or rejected is not appropriate; one should seek rather to evaluate the "goodness" of the predictions and the errors associated with the model. Schruben (1980) also stated that the development of a strictly valid model of a nontheoretical process is impossible. Reckhow (1981), in a philosphical analysis of model verification, stated that the testing of models is an inductive process and that verification, which he defined as the ascertainment of truth, is inconsistent with the inductive logic of scientific research. Wright (1972), in a review of ecosystem models, agreed that predictive models could not be invalidated. House (1974) hypothesized that the world is so complex that attempts to completely validate forecasting models are futile.

7. Regardless of whether or not one can state that a model is, or is not, valid, methods have been put forth to compare model output to measured values. Graphical techniques are often used; i.e., a particular variable is plotted through time as predicted and as measured, and the plots are compared qualitatively. In addition to qualitative tests, a number of quantitative tests have been proposed. Some of the tests appear to have been developed especially for model testing; these include Theil's (1961) inequality coefficient, Kapoor's (1968) inequality coefficient, a reliability index for models (Leggett and Williams 1981), and a procedure for simulation model acceptance (Schruben 1980).

Other quantitative tests of model validity are based on statistical measures which generally show whether or not two samples came from the same population. (Table 1 lists some of these.) Some of the statistical tests are appropriate for distributions of residuals, others for comparison of frequency distributions; some are for deterministic models, and others for stochastic models; some of the tests are parametric, while others are nonparametric. As with terminology, there does not seem to be general agreement on particular tests, and tests recommended by some authors may be rejected by others. For example, according to Wright (1972), "Using either regression or factor analysis to validate computer simulation models is absurd"; concerning tests of selected measures from distributions, he wrote "At worst, such tests are totally improper; at best, they destroy the structure-in-time of the trajectories being contrasted."

Table 1

A Partial List of Statistical Tests for Comparing Model Predictions and Measured Data*

Analysis of variance	Regression analysis
Chi-square	Relative error
Comparison of means	Root-mean-square error
Factor analysis	1 sample t-test
F-test	2 sample t-test
Kendall tau	Sign test
Kolmogorov-Smirnov test	Spearman rho
Mann-Whitney test	Spectral analysis
Normalized mean error	Wald-Wolfowitz test
Pearson product moment correlation coefficient	Wilcoxon test

* From Mihram (1972), Reckhow (1981), Wright (1972), Thomann (1980), Gordon (1981), and TRC (1981).

8. A workshop on verification of water quality models was convened by the Environmental Protection Agency in 1979. The proceedings from the workshop (U. S. Environmental Protection Agency (EPA) 1980) are especially apropos to the present model evaluation. The members of the workshop recommended the review of software code and the use of internal automated checks for evaluating computer programs. They also generally agreed that an adequate model evaluation would consist of comparing computed model results to a set of water quality data other than the calibration data set. Although they encouraged the use of statistical techniques, they did not recommend any statistics, nor did they believe that statistical techniques should supersede engineering judgement.

PART III: RATIONALE AND EVALUATION METHODS

Model Objectives

9. Innis (1975) and Swartzman (1979) argued that evaluation criteria should depend on model objectives. In agreement with their argument, the objective of developing the CE-QUAL-R1 model may be stated thus: to provide CE District and Division offices with a means of studying preimpoundment and postimpoundment water quality problems and the effects of reservoir operation on water quality. Examples of functions that the model can perform include:

- a. Determine onset, extent, and duration of thermal stratification.
- b. Locate selective withdrawal ports required to meet a downstream water quality objective.
- c. Determine the effect of structural modifications on water quality.
- d. Predict the development of anoxic conditions.
- e. Provide information concerning algal blooms.
- f. Isolate factors limiting algal growth.
- g. Predict effects of storm events on inpool and release water quality.
- h. Determine effects of upstream land use on inpool and release water quality.
- i. Determine effects of project operation changes such as:
  - (1) Altered release level.
  - (2) Change in minimum or maximum release rate.
  - (3) Changes in pool elevation.
  - (4) Destratification.

10. CE-QUAL-R1 will be used as a management tool, often on reservoirs that are only in the planning stage. The model must therefore be general enough to allow for its use in simulating a variety of impoundments, planned or in existence, with a host of possible operational plans. CE-QUAL-R1 fulfills that requirement because it is not a model per se, using the same set of initial conditions, coefficients, and

updates for all possible reservoirs. It is rather a model framework which becomes a model for a particular waterbody after it has incorporated the initial conditions, coefficients, and descriptions that are characteristic of a particular site.

Evaluation Objective

11. With the above two model objectives in mind, the goal of the evaluation process will be to supply the best possible tool, within the assumptions specified for CE-QUAL-R1, for reservoir water quality management. The process will not, as has been argued by Goodall (1972), Schruben (1980), Reckhow (1981), Wiegert (1975), House (1974), and others, tell if CE-QUAL-R1 is or is not valid. There are unresolved questions about the validity of the predictions of any model that predicts numerous variables in a number of layers and whose predictions may not fall within some confidence band. Suppose, for example, predictions of oxygen for 1 year were compared to monthly observed data and all comparisons were satisfactory except those predicted for May. If one considers the predictions to be satisfactory 11 out of 12 times, one assumes that there is some sort of self-correcting mechanism built into the model concerning oxygen prediction, for the predicted value at one point in time depends on the previously predicted values. Would the predictions be considered valid only through April?

12. Suppose, in another case, that a model predicts both oxygen and algae. Suppose further, that comparisons show that oxygen predictions are satisfactory but algal predictions are not. Can the model be considered okay for predicting oxygen? Because the oxygen predictions are in part based on concentrations of algae which are not satisfactory, the model may be predicting the correct oxygen values for the wrong reason.

13. With the above arguments in mind, and in agreement with the authors cited above, this author does not believe that the evaluation process can supply a model that has been completely verified, or one that is or is not valid. He offers, instead, an evaluation of CE-QUAL-R1 that will improve predictions by (a) testing alternate

algorithms for the same process, or (b) testing the results achieved using alternate processes or variables. The results of the evaluation must then be transferred to the managers who intend to use model predictions, because the ultimate judgement of a model depends on the objectives of a particular study. As with most other model evaluations (see paragraphs 5 and 6), two main processes will be used for the evaluation: the first tests the software code; the second examines model predictions.

14. The term calibration will be used in this report to mean the process of adjusting a set of coefficients by comparing model predictions to measured values for a data set representing a particular reservoir for a particular period of time. The term verification will be used to mean the process of comparing model predictions to measured values using a data set representing the same reservoir used for calibration, but for a different time period. The verification data set must retain the same coefficients as were used for the calibration exercise.

Evaluation of Software

15. The origin of CE-QUAL-R1 dates back to 1972 (Environmental Laboratory 1982). Since that time numerous changes have been made to the code. Due to the size of the model and the number of interactions among variables, some of the changes may have inadvertently caused problems in other parts of the model. Some errors may be very difficult to find because all of the code is not necessarily executed during every simulation. Among others, the following methods are proposed for software evaluation.

a. Check the equations for correct dimensionality.

b. Ensure that model predictions are numerically stable. Predictions should not oscillate more than measurements found in nature from one time step to the next; in addition, predictions should not vary appreciably when the time step is varied.

c. Test for conservation of mass. The test should be made for both conservative and nonconservative substances.

d. Check initial values for zero entries. Occasionally a variable may not be given a correct initial value, in which case the computer supplies a zero value. The zero value may allow computations concerning the variable to

be carried out, but the results are incorrect. A method supplied for the Boeing Mainstream-EKS interactive time-sharing computer system allows the checking of all variables to ensure that initial values were set.

e. As was suggested by Mihram (1972) and Lawler (1980), constant values for a conservative substance can be used for inflowing concentrations, which should force predicted values in the water column to approach these constant values. Increased flows should cause the constant values to be reached more quickly. Care must be taken as this test can apply to the entire water column only during isothermal conditions. The mixing coefficients can be changed to ensure complete mixing.

f. Thoroughly check problems reported by individuals or groups which are using CE-QUAL-R1.

Evaluation of Model Predictions

Graphical comparisons

16. Models are here evaluated in both a qualitative and quantitative fashion. Qualitatively, the interactive graphics package (Environmental Laboratory 1982) is used, with predicted and measured values graphed together. Figure 1 is an example of graphical output.

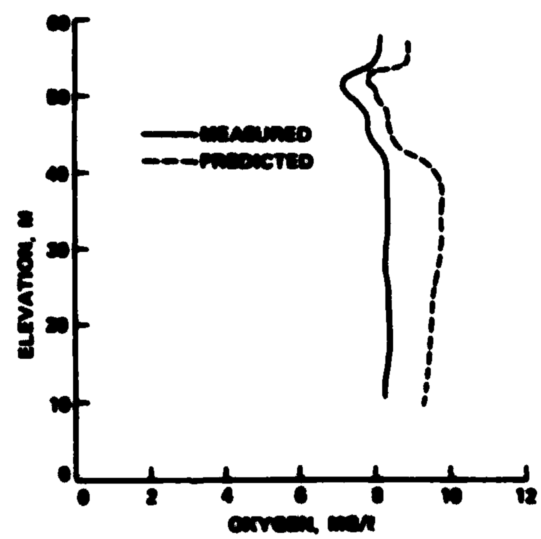
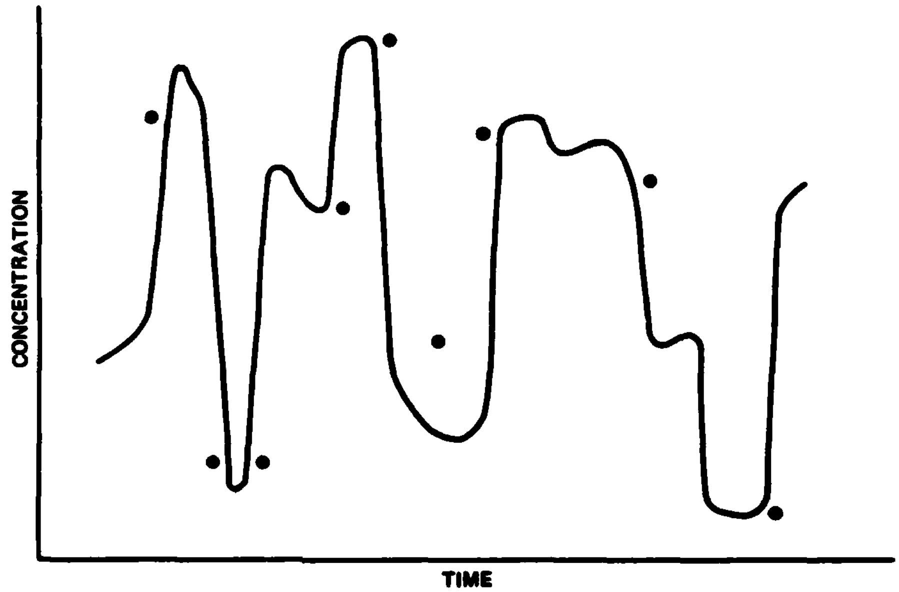


Figure 1. An example of graphical output comparing measured and predicted values (DeGray Reservoir oxygen profile on 1 May 1979)

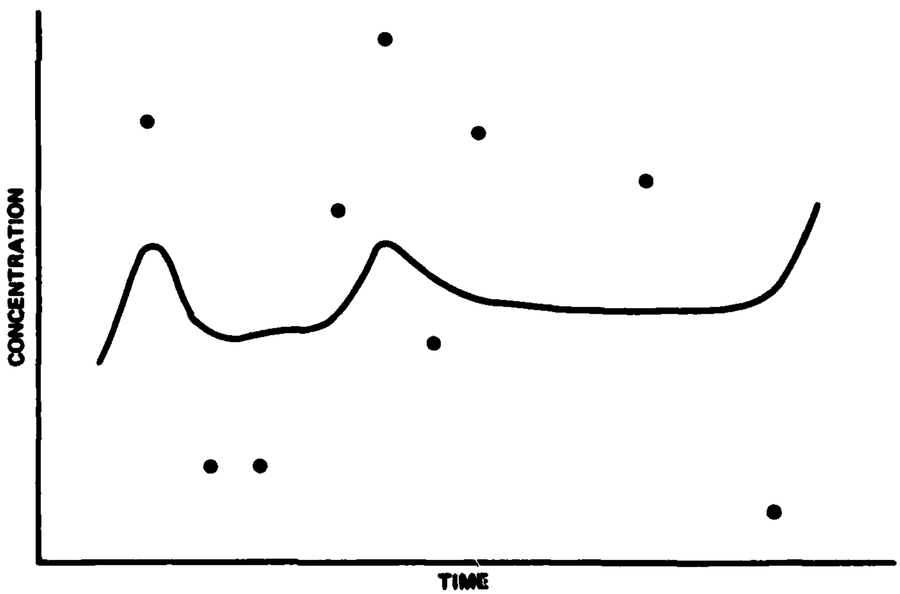
Graphical comparisons are used in addition to statistical analysis because statistics can often be misleading. Consider, for example, Figure 2. In both figures the solid circles represent measured values and the line represents model predictions. The lines in the two figures represent different algorithms for the same process. Even though the comparisons in Figure 2a appear to be better, most statistical analyses would show that the algorithm represented in Figure 2b is superior. The reason for this apparent anomaly is that, although the measured points in Figure 2a are close to the predicted line horizontally along the time axis, they are not so close as in Figure 2b when measured vertically along the concentration axis at common points in time. Since most statistical analyses compare the concentrations of measured and predicted values at the same points in time, the line in Figure 2b actually is statistically a better representation of measured values.

Statistical analyses

17. Although conclusions about the adequacy of model predictions for a particular variable can be made when viewing a graph, the number of variables and the number of layers for which measured data are available could be so great as to preclude adequate judgement of the total model. For these cases statistical analyses would be useful. Statistical packages can be used to test which of two algorithms for a particular process is a better predictor or which of a number of sets of coefficients produce simulation curves which most closely correspond to observed data. A statistics program is available for evaluating CE-QUAL-R1. It contains the following statistics: (a) reliability index (Leggett and Williams 1981); (b) paired t-test for means (Sokal and Rohlf 1969); (c) normalized mean error (Gordon 1981, see also Wlosinski 1982); and (d) coefficients for the linear regression equation for plotting observed versus predicted values (Thomann 1980). Equations for these statistics can be found in Appendix A. Note that these statistical equations can be applied either to data collected at a single point in time, or to data collected at a number of times throughout a sampling period. In this way the evaluation of predicted time series or trends can be accomplished.



a. Algorithm 1 results compared to measured values



b. Algorithm 2 results compared to measured values

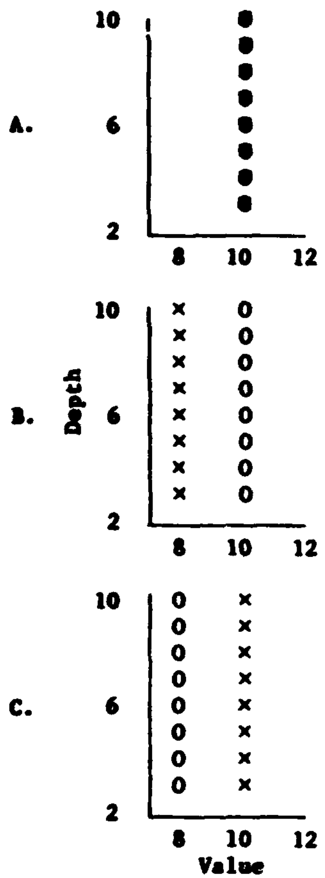
Figure 2. Example of a comparison of results of two models to the same data set. The solid line represents predicted values; the circles represent measured values

18. Results from statistical analysis can be misleading, so the user is cautioned to view graphs of simulation results in addition to using the statistical package. To help familiarize the user with statistical results and to present some possible problems, a series of graphs comparing observed and predicted values is presented in Figure 3. The first graph (A) represents one case of perfect prediction. In such cases the value for the normalized mean error is 0.0, and for the reliability index it is 1.0; for the paired t-test for means, the computed T is undefined since the denominator in the equation equals zero.

19. Other cases are possible where the value for T is undefined but where predicted and observed values are not equal. This is illustrated in the next nine graphs (B-J) in Figure 3. In still other cases, as shown in graphs K and L, a computed T may equal 0.0, signifying that the means are the same, but individual predictions are not the same as observed values. If the user based his judgment of the model solely on this statistic, he would not draw correct conclusions.

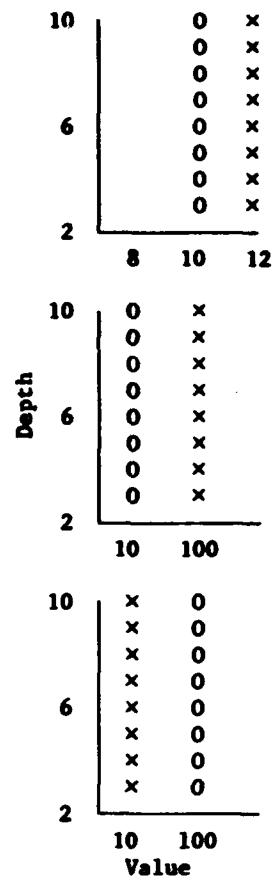
20. The coefficients a, b, and r^2 for the linear equation are undefined in graphs A-J because there is only one value for the x axis and at least two values are needed for the computation. For the coefficients for the linear equation to represent a case of perfect prediction, a must equal 0.0, b must equal 1.0, and r^2 must equal 1.0. It is possible to have one or two of the coefficients correct and still have predicted values which are not equal to measured values; graph L is an example of this problem.

21. In graphs B-D the differences between the predicted and observed values are equal, but the values for the reliability index and the normalized mean error are not necessarily the same. For both of these statistics the values are scale-variant; that is, the same numerical difference between their observed and predicted values will produce a smaller calculated value as the numbers being compared become greater. In the case of the normalized mean error, scale variance depends in part on the observed values, since they occur in the denominator; thus, the value for the normalized mean error is the same in graphs B and D, but different from the value in C. This is not the case for the reliability



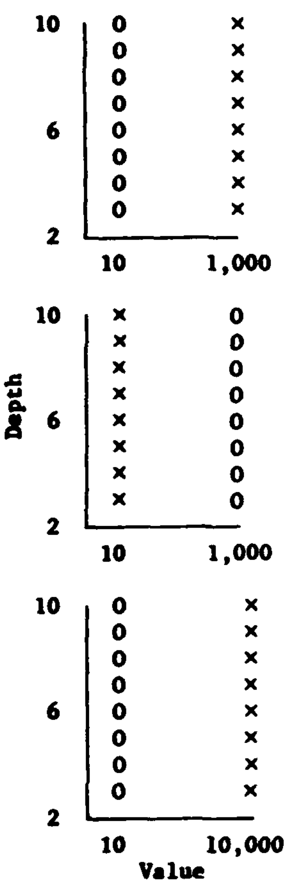
	Observed(O) Mean	Predicted(X) Mean	T	Reliability Index	Normalized Mean Error	Linear Equation a	Linear Equation b	Linear Equation r^2
A.	10.0	10.0	U	1.0	0.0	U	U	U
B.	10.0	8.0	U	1.25	20.0	U	U	U
C.	8.0	10.0	U	1.25	25.0	U	U	U

Figure 3. Graphs comparing observed (O) and predicted (X) values. Undefined values are represented by U (Sheet 1 of 4)



	Observed(0) Mean	Predicted(X) Mean	T	Reliability Index	Normalized Mean Error	Linear Equation a	b	r^2
D.	10.0	12.0	U	1.20	20.0	U	U	U
E.	10.0	100.0	U	10.0	900.0	U	U	U
F.	100.0	10.0	U	10.0	90.0	U	U	U

Figure 3. (Sheet 2 of 4)



	Observed(0) Mean	Predicted(X) Mean	T	Reliability Index	Normalized Mean Error	Linear Equation a	b	r^2
G.	10.0	1,000.0	U	100.0	9900.0	U	U	U
H.	1,000.0	10.0	U	100.0	99.0	U	U	U
I.	10.0	10,000.0	U	1,000.0	99,900.0	U	U	U

Figure 3. (Sheet 3 of 4)

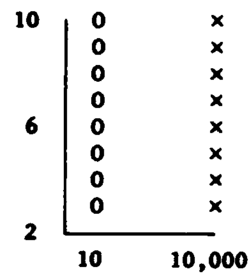
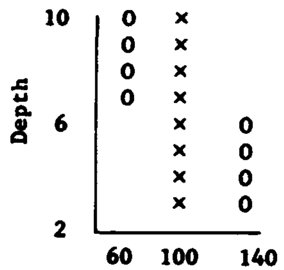
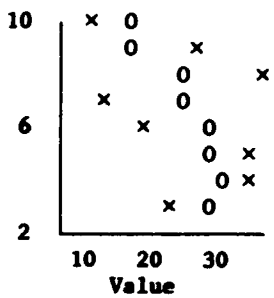
		Observed(0) Mean	Predicted(X) Mean	T	Reliability Index	Normalized Mean Error	Linear Equation a	Linear Equation b	Linear Equation r^2
J.		10,000.0	10.0	U	1,000.0	99.0	U	U	U
K.		100.0	100.0	0.0	1.54	47.6	100.0	0	U
L.		17.5	17.5	0.0	2.15	52.9	0.0	1.1	0.27

Figure 3. (Sheet 4 of 4)

index, so graphs B and C produce the same result which is different from D's. Graphs E-J are presented to show the results of different statistics when observed and predicted values are one, two, and three orders of magnitude apart. Because the reliability index shows an increasing value which does not depend on whether the observed or predicted value is greater, it appears to be the best statistic for aggregating results.

22. But to use these tests correctly, a number of assumptions must be satisfied (Sokal and Rohlf 1969). First, samples should be collected at random. This is rarely done in collecting water quality data, for it is more important to be able to gain information, for purposes other than model evaluation, about the system under study by sampling at set intervals of time and at uniform distributions through space; in addition, the majority of the data are taken during daylight hours. Second, the samples should be independent of one another. This assumption is violated because the model's prediction at one point in time depends on previous values. In addition, the statistical tests are valid only if the samples have homogeneity of variances and are normally distributed and, in the normal case of regression, if the independent variable is measured without error.

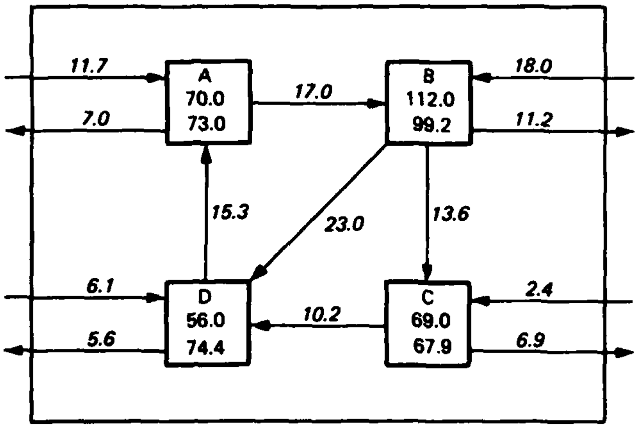
23. Tests and possible alternatives for these assumptions are available (see for example, Sokal and Rohlf 1969). Some of the adjustments may include changing the basic design of the experimental program, or not using all of the collected data. Rather than spending time and resources in checking these assumptions or deleting data to make sure that the statistical results are absolutely valid, the statistics are here used as a tool in comparing alternative formulations. A listing of the statistical package and information concerning its use are included in Appendix B.

24. All of the statistical tests which are proposed compare one predicted value against one observed value, but most reservoir data sets have more than one station at which data were collected. The model can be run stochastically, a process which produces a series of values for each variable at each depth for each time step. However, the cost to run the model stochastically to test a number of algorithms for the

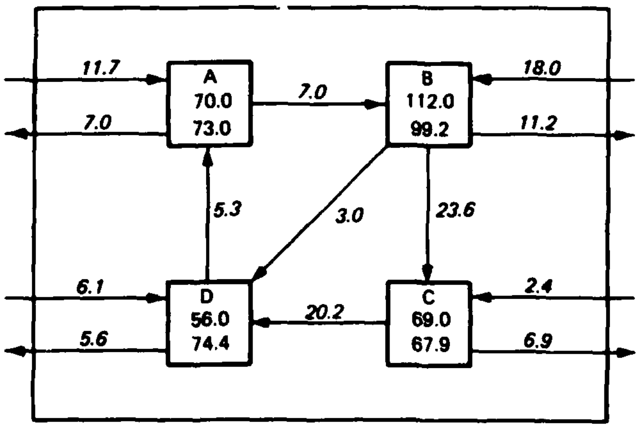
same process, or to add or delete processes or variables, would be prohibitive. Also, creating a value that is supposed to be measured, either by arithmetic averaging or averaging by volume weighting, could produce a data set that is not realistic. For example, suppose that the water entering a reservoir is colder than the reservoir proper. The time is early spring, the reservoir is well mixed, and the water is entering as a plug flow, warming as it moves through the reservoir. Because the reservoir is deeper near the dam, averaging the temperature at different stations would produce a data set that has cooler surface water over a warmer hypolimnion. Physically this does not happen, and using these data may result in the acceptance of inferior algorithms. For the proposed evaluation, predicted results usually come from running the model in the deterministic mode, and comparisons are made to data collected at a single station, usually in the deepest part of the reservoir. Occasionally the model will be run in a stochastic fashion, and for specific variables at certain depths the results will be graphed with measured values at all stations.

Comparing measured and predicted flux values

25. Most of the literature concerning the comparison of model predictions and measured values deals with the comparison of the mass or concentration of variables. However, it is possible to predict the same values for state variables with very different fluxes (the term flux refers to the amount of materials transferred between model variables; e.g., the amount of phytoplankton ingested by zooplankton). An example of this is shown in Figure 4. In each model there are four compartments, with the values for the initial conditions listed above the predicted values after one time step. For both models, the predicted values were the same even though the fluxes were different. The predicted values were calculated using the equations listed in Table 2 and the coefficients and driving variables listed in Table 3. This same type of problem was shown by Scavia (1980) to occur when using a model of Lake Ontario. Even in the case where different data sets are used



MODEL I



MODEL II

Figure 4. An example of calibrating two models having the same initial and final values but different flux values

Table 2

Equations Representing the Systems Used in Figures 4 and 5

$$\frac{dA}{dt} = -Ac_1v_1 + Dc_4v_4 - Av_6 + I_A$$

$$\frac{dB}{dt} = Ac_1v_1 - Bc_2v_2 - Bc_5v_5 - Bv_6 + I_B$$

$$\frac{dC}{dt} = Bc_2v_2 - Cc_3v_3 - Cv_6 + I_C$$

$$\frac{dD}{dt} = Bc_5v_5 + Cc_3v_3 - Dc_4v_4 - Dv_6 + I_D$$

where

t equals time

A , B , C , and D represent mass of variables

c_1 , c_2 , c_3 , c_4 , and c_5 are coefficients

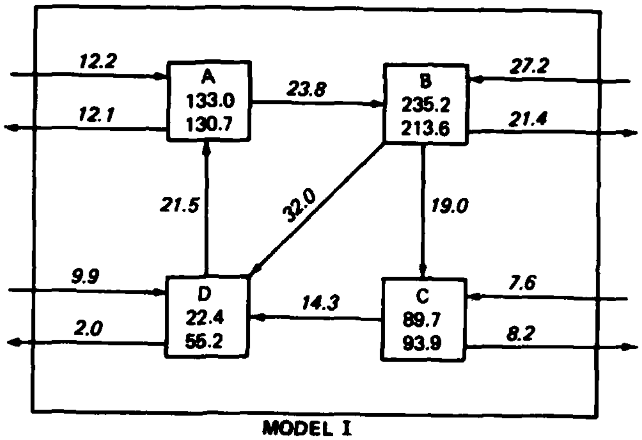
v_1 , v_2 , v_3 , v_4 , v_5 , and v_6 are driving variables

I_A , I_B , I_C , and I_D represent the mass entering respective compartments from outside the system

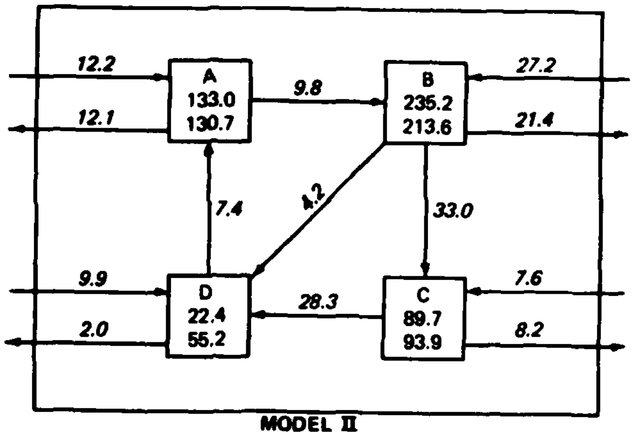
Table 3

Coefficients and Driving Variables Used for the Systems Represented in Figures 4 and 5

Coefficients	Model I	Model II	Driving Variables	Calibration	Verification
c_1	0.2429	0.10	v_1	1.0	0.7368
c_2	0.160	0.2776	v_2	0.7589	0.506
c_3	0.0157	0.03114	v_3	9.4	10.12
c_4	1.70	0.5889	v_4	0.1607	0.5635
c_5	5.70	0.7440	v_5	0.0360	0.0239
			v_6	0.10	0.091



MODEL I



MODEL II

Figure 5. An example of verifying two models having the same initial and final values but different flux values

for calibration and verification, there is no way of telling if the second data set is different enough to allow for the discovery of the flux problem. Suppose, for example, that a second data set was available to be used for verification (Figure 5). Since the two models of the same system had different coefficients and therefore different fluxes, only one of the models would be expected to accurately predict the measured values for the verification exercise. The verification data set had different driving variables (Table 3) and initial conditions (Figure 5)

from the calibration data set. The same model, outlined in Table 2, and the same coefficients (Table 3), were used with the second data set. As can be seen in Figure 5, different fluxes were predicted, but again the two models predicted the same values after a single time step.

26. This example illustrates that one cannot depend solely on comparing predicted versus measured quantities of state variables when calibrating or verifying models. In order to ensure reliable models for a particular system, calibration and verification procedures should include comparisons of measured versus predicted flux values as well as of measured versus predicted quantities for state variables.

27. For CE-QUAL-R1, a peripheral package has been developed which provides estimates of the flux values used to calculate values for variables for the next time step. The flux values reported are estimates; this is because in all cases for the flux package an Euler technique is used to solve the equations, whereas most variables included in the full water quality model are solved using a 2-step (predictor-corrector) Euler procedure. The connection between CE-QUAL-R1 and the flux package is a file created during the simulation. The name of the file is included on the FILES card (Environmental Laboratory 1982) after the names for the plot files. Information concerning the use of the flux package is included in Appendix C. A computer listing is not included because the computer code will be changed as new algorithms concerning processes replace present formulations.

28. The methods for model evaluation discussed in this report can be used when the model CE-QUAL-R1 is applied to either an existing or a proposed reservoir. In the case of a preimpoundment study, however, the data for use in model calibration and/or verification will be drawn from other nearby reservoirs judged to be sufficiently similar to the proposed project that observations from these other systems are representative of the reservoir under study. Otherwise, evaluation of model predictions must rely strictly on scientific and engineering judgment. The reader is referred to the reports of Fort et al. (1977, 1979) and Thornton et al. (1976, 1977) as examples of uses of developmental versions of CE-QUAL-R1 in preimpoundment investigations.

REFERENCES

Bedford, Keith W., and Babajimopoulos, Christos. 1980. "Verifying Lake Transport Models with Special Statistics, 106(HY1):21-37.

Caswell, H. 1976. "The Validation Problem," Pages 313-325 in B. C. Patten, ed., Systems Analyses and Simulation in Ecology, Vol 4, Academic Press, New York.

Environmental Laboratory. 1982. "CE-QUAL-R1: A Numerical One-Dimensional Model of Reservoir Water Quality; User's Manual," Instruction Report E-82-1, U. S. Army Engineer Waterways Experiment Station, Vicksburg, Miss.

Ford, D. E., Thornton, K. W., Ford, W. B.,III, and Lessem, A. S. 1979. "Water Quality Evaluation of Proposed Twin Valley Lake, Wild Rice River, Minnesota," Technical Report EL-79-5, U. S. Army Engineer Waterways Experiment Station, Vicksburg, Miss.

Ford, D. E., Thornton, K. W., and Robey, D. L. 1977. "Preliminary Water Quality Evaluation of a Lower Pool Elevation for Proposed LaFarge Lake, Wisconsin," Miscellaneous Paper Y-77-2, U. S. Army Engineer Waterways Experiment Station, Vicksburg, Miss.

Gentil, S., and Blake, G. 1981. "Validation of Complex Ecosystem Models," Ecological Modelling, 14:21-38.

Goodall, D. W. 1972. "Building and Testing Ecosystem Models," Pages 173-194 in J. N. R. Jeffers, ed., Mathematical Models in Ecology, Blackwell Science Publications, Oxford, England.

Gordon, John A. 1981. "LARM Two-Dimensional Model: An Evaluation," ASCE Journal of the Environmental Engineering Division, 107(EE5): 877-886.

Hall, C. A. S., and Day, J. W., Jr., 1977. "Systems and Models: Terms and Basic Principles," Pages 6-36 in C. A. S. Hall and J. W. Day, Jr., eds., Ecosystem Modeling in Theory and Practice: An Introduction with Case Histories, John Wiley and Sons, New York.

House, Peter W. 1974. "Diogenes Revisited--the Search for a Valid Model," Simulation, 23(4):117-125.

Innis, G. S. 1975. "The Role of Total Systems Models in the Grassland Biome Study," in B. C. Patten, ed., Systems Analysis and Simulation in Ecology, Vol III, Academic Press, New York.

Kapoor, U. K. 1968. "On the Validation of Simulation Experiments: A Review of Existing Techniques and a Proposed Technique for the Wisconsin River Water Quality Simulation Model," M.S. Thesis, University of Wisconsin, Madison, 28 pp. (As cited in M. Garratt. 1975. "Statistical Techniques for Validating Computer Simulation Models," US/IBP Grassland Biome Technical Report No. 286, National Res. Ecology Laboratory, Colorado State University, Ft. Collins, 68 pp.)

Keeley, J. W., Mahloch, J. L., Barko, J. W., Gunnison, D., and Westhoff, J. D. 1978. Identification and Assessment of Environmental Quality Problems and Research Program Development," Technical Report E-78-1, U. S. Army Engineer Waterways Experiment Station, Vicksburg, Miss.

Lawler, John P. 1980. "Modeling Framework and Software Validation," in Workshop on Verification of Water Quality Models, EPA Environmental Research Laboratory, Athens, Ga.

Leggett, R. W., and Williams, L. R. 1981. "A Reliability Index for Models," Ecological Modelling, 13:303-312.

Mankin, J. B., O'Neill, R. V., Shugart, H. H., and Rust, B. W. 1977. "The Importance of Validation in Ecosystem Analysis," Pages 63-71 in G. S. Innis, ed., New Directions in the Analysis of Ecological Systems, Part 1, The Society for Computer Simulation, La Jolla, Calif.

Mihram, G. Authur. 1972. "Some Practical Aspects of the Verification and Validation of Simulation Models," Operational Research Quarterly, 23(1):17-29.

Miller, D. R. 1974. "Sensitivity Analysis and Validation of Simulation Models," Journal of Theoretical Biology, 48:345-360.

Nolan, R. L. 1972. "Verification/Validation of Computer Simulation Models," Pages 1254-1265 in Proceedings of the 1972 Summer Computer Simulation Conference, Simulation Councils, La Jolla, Calif.

O'Neill, R. V. 1975. "Management of Large-Scale Environmental Modeling Projects," Pages 251-282 in C. S. Russell, ed., Ecological Modeling in a Resource Management Framework, Resources for the Future, Inc., Washington, D. C.

Orlob, G. T. 1975. "Present Problems and Future Prospects of Ecological Modeling," Pages 283-312 in C. S. Russell, ed., Ecological Modeling in a Resource Management Framework, Resources for the Future, Inc., Washington, D. C.

Reckhow, Kenneth H. 1981. "Model Verification: A Philosophical and Statistical Analysis," Presented at the 1981 Conference of the American Water Resources Association, Atlanta, Ga.

Scavia, D. 1980. "The Need for Innovative Verification of Eutrophication Models," in "Workshop on Verification of Water Quality Models," EPA Environmental Research Laboratory, Athens, Ga.

Schruben, Lee W. 1980. "Establishing the Credibility of Simulations," Simulation, 101-105.

Sokal, R. R., and Rohlf, F. James. 1969. Biometry. W. H. Freeman and Company, San Francisco.

Swartzman, Gordon. 1979. "Evaluation of Ecological Simulation Models," in G. P. Patil and M. L. Rosenzweig, eds., Contemporary Quantitative Ecology and Related Econometrics, International Cooperative Publishing House, Missouri.

Theil, H. 1961. Economic Forecasts and Policy, 2nd ed, North Holland Publishing Co., Amsterdam, 567 pp.

Thomann, R. V. 1980. "Measures of Verification," in Workshop on Verification of Water Quality Models, EPA Environmental Research Laboratory, Athens, Ga.

Thornton, K. W., Ford, D. E., Hall, R. W., Eley, R. L., and Robey, D. L. 1977. "Water-Quality Evaluation of a Lower Pool Elevation for Proposed Arcadia Lake, Oklahoma," Technical Report Y-77-3, U. S. Army Engineer Waterways Experiment Station, Vicksburg, Miss.

Thornton, K. W., Ford, D. E., and Robey, D. L. 1976. "Preliminary Evaluation of Water Quality of Proposed LaFarge Lake, Kickapoo River, Vernon County, Wisconsin," Miscellaneous Paper Y-76-5, U. S. Army Engineer Waterways Experiment Station, Vicksburg, Miss.

TRC-Environmental Consultants. 1981. "Validation of Plume Models Statistical Methods and Criteria," EA-1673-SY, Electric Power Research Institute, Palo Alto, Calif.

U. S. Environmental Protection Agency (EPA). 1980. "Workshop on Verification of Water Quality Models," Environmental Research Laboratory, Athens, Ga.

Weatherbe, D. G. 1976. "A Dynamic Water Quality Simulation Model for the Thames River, in Proceedings of the Conference on Environmental Modeling and Simulation, Environmental Protection Agency No. 600/9-76-016.

Wiegert, R. G. 1975. "Simulation Models of Ecosystems," Pages 311-338 in R. F. Johnson, ed., Annual Review of Ecology and Systematics, Vol 6, Annual Reviews Inc., Palo Alto, Calif.

Wlosinski, J. H. 1982. "A Discussion of the Paper 'LARM Two-Dimensional Model: An Evaluation,'" ASCE Journal of the Environmental Engineering Division, 108(3):605-606.

Wright, Richard D. 1972. "Validating Dynamic Models. An Evaluation of Tests of Predictive Power," Pages 1286-1294 in Proceedings of the 1972 Summer Computer Simulation Conference, Simulation Councils, La Jolla, Calif.

APPENDIX A: STATISTICAL EQUATIONS

1. Let A_{tn} equal the measured value at the n^{th} depth during the t^{th} sample period for a particular variable, and let P_{tn} equal the value for the corresponding predicted variable where

$t = 1,\ldots,T$ (total number of sampling periods for a variable)

$n = 1,\ldots,N$ (total number of depths sampled for each sampling period)

N = total number of observed samples for all depths for all sampling periods

2. The reliability index RI (Leggett and Williams 1981) is defined as:

$$RI_t = \frac{1 + \sqrt{\frac{1}{N} \sum_{n=1}^{N} \left[\frac{1 - (A_{tn}/P_{tn})}{1 + (A_{tn}/P_{tn})}\right]^2}}{1 - \sqrt{\frac{1}{N} \sum_{n=1}^{N} \left[\frac{1 - (A_{tn}/P_{tn})}{1 + (A_{tn}/P_{tn})}\right]^2}}$$

for a sampling period or

$$RI = \frac{1 + \sqrt{\frac{1}{\Sigma N} \sum_{t=1}^{T} \sum_{n=1}^{N} \left[\frac{1 - (A_{tn}/P_{tn})}{1 + (A_{tn}/P_{tn})}\right]^2}}{1 - \sqrt{\frac{1}{\Sigma N} \sum_{t=1}^{T} \sum_{n=1}^{N} \left[\frac{1 - (A_{tn}/P_{tn})}{1 + (A_{tn}/P_{tn})}\right]^2}}$$

for all sampling periods for a particular variable.

The paired t test for means B is calculated as

$$B_t = \frac{\left(\sum_{n=1}^{N} A_{tn}/N\right) - \left(\sum_{n=1}^{N} P_{tn}/N\right)}{\sqrt{\frac{N \sum_{n=1}^{N}(A_{tn} - P_{tn})^2 - \left(\sum_{n=1}^{N} A_{tn} - P_{tn}\right)^2}{N^2(N - 1)}}}$$

for a sampling period or

$$B = \frac{\left(\sum_{t=1}^{T} \sum_{n=1}^{N} A_{tn}/\Sigma N\right) - \left(\sum_{t=1}^{T} \sum_{n=1}^{N} P_t/\Sigma N\right)}{\sqrt{\frac{\Sigma N \sum_{t=1}^{T} \sum_{n=1}^{N} (A_{tn} - P_{tn})^2 - \left[\sum_{t=1}^{T} \sum_{n=1}^{N} (A_{tn} - P_{tn})\right]^2}{(\Sigma N)^2(\Sigma N - 1)}}}$$

for all sampling periods for a particular variable.

3. The normalized mean error NME (Gordon 1981; see also Wlosinski 1982) is calculated as

$$NME_t = \frac{\sum_{n=1}^{N}\left(\frac{\lfloor P_{tn} - A_{tn} \rfloor}{A_{tn}}\right) 100}{N}$$

for a sampling period or

$$NME = \frac{\sum_{t=1}^{T} \sum_{n=1}^{N}\left(\frac{\lfloor P_{tn} - A_{tn} \rfloor}{A_{tn}}\right) 100}{\Sigma N}$$

for all sampling periods for a particular variable.

4. The final statistical test is a regression analysis of the relationship between predicted and measured values. The statistical test gives estimates of a and b in the equation

$$\bar{P}_{tn} = a + b\bar{A}_{tn}$$

which could then be compared with the equation for perfect prediction, where a equals 0.0 and b equals 1.0, using the Students t distribution. In addition, the square of the correlation coefficient (r^2), which is a measure of the variance accounted for between observed and predicted values, can be calculated.

5. Calculate

$$\Sigma A = \sum_{t=1}^{T} \sum_{n=1}^{N} A_{tn}$$

$$\Sigma P = \sum_{t=1}^{T} \sum_{n=1}^{N} P_{tn}$$

$$\Sigma A^2 = \sum_{t=1}^{T} \sum_{n=1}^{N} A_{tn}^2$$

$$\Sigma P^2 = \sum_{t=1}^{T} \sum_{n=1}^{N} P_{tn}^2$$

$$\Sigma AP = \sum_{t=1}^{T} \sum_{n=1}^{N} A_{tn}P_{tn}$$

$$\bar{A} = \frac{\Sigma A}{\Sigma N}$$

$$\bar{P} = \frac{\Sigma P}{\Sigma N}$$

$$FA = \frac{\Sigma A^2 - \frac{(\Sigma A)^2}{\Sigma N}}{(\Sigma N) - 1}$$

$$FP = \frac{\Sigma P^2 - \frac{(\Sigma P)^2}{\Sigma N}}{(\Sigma N) - 1}$$

$$FAP = \frac{\Sigma AP - \frac{\Sigma A \Sigma P}{\Sigma N}}{(\Sigma N) - 1}$$

The coefficients b and a are calculated from the equations

$$b = \frac{FAP}{FA}$$

$$a = \bar{P} - b\bar{A}$$

Further calculate

$$SD = [(\Sigma N) - 1]b^2 FA$$

$$ST = [(\Sigma N) - 1]FP$$

$$S = \frac{ST - SD}{(\Sigma N) - 2}$$

$$Vb = \frac{S}{[(\Sigma N) - 1]FA}$$

$$Va = \frac{S\{[(\Sigma N) - 1]FA + \bar{A}^2 \Sigma N\}}{\Sigma N[(\Sigma N) - 1]FA}$$

The null hypothesis NH , that the computed slope equals one, is tested with

$$NH = \frac{b - 1}{\sqrt{Vb}}$$

with $(\Sigma N) - 2$ degrees of freedom. The null hypothesis, that the intercept equals zero, is tested with

$$NH = \frac{a}{\sqrt{Va}}$$

with $(\Sigma N) - 2$ degrees of freedom. The correlation coefficient r^2 equals

$$r^2 = \frac{SD}{ST}$$

APPENDIX B: STATISTICAL PACKAGE

1. As with CE-QUAL-R1, the statistical package resides on the Boeing Mainstream-EKS interactive time-sharing computer system. A user must have his own account number and should have some knowledge of Boeing procedures. Because of the large amount of data generated by the CE-QUAL-R1 model, two executions are needed. The first execution is used only to delete predicted data on dates when no measured data are available. To execute this program, prepare a file as follows for use by the SUBMIT directive:

```
GRAXEQ,CM320000,T300,P1.
USER,ID,PASWORD.
GET,GRAOBJ/UN=CEROB5.
GET,TAPE5=LDATE.
GET,TAPE89=PLDG14.
FILE,TAPE6,FF=YES.
LOADXEQ,F=GRAOBJ,M=FULL/MAPGRA.
EXIT,U.
REPLACE,MAPGRA.
EXIT,U.
REPLACE,TAPE6=GRADAT.
EXIT,U.
REPLACE,OUTPUT=PUTOUT1.
EXIT,U.
COST,LO=F.
EXIT,U.
DAYFILE,DFXGRA.
REPLACE,DFXGRA.
```

2. Names that are underlined can be changed at the users discretion. File LDATE contains the dates on which measured data are available. One date should be in the first six columns of each line: the first two columns represent the last two digits of the year, columns three and four contain the number of the month, and columns five and

six contain the day of the month. File PLDG14 is the same file as is used by the interactive graphics package (see Environmental Laboratory 1982).

3. Upon satisfactory completion of the execution, four files will be created and permanently stored. File MAPGRA contains the storage location map. File GRADAT is the output file that will be used in the next execution which will perform the statistical analysis. File PUTOUT1 contains information concerning problems during execution. File DFXGRA is the dayfile which describes the execution.

4. To execute the statistical package, the following file is needed.

```
STSTXEQ,CM320000,T15,P01.
USER,ID,PASWORD.
GET,STSTOBJ/UN=CEROB5.
GET,TAPE22=VD794.
GET,TAPE23=GRADAT.
GET,TAPE6=STSWICH.
FILE,TAPE7,FF=YES.
LOADXEQ,F=STSTOBJ,M=FULL/MAPSTST.
EXIT,U.
REPLACE,MAPSTST.
EXIT,U.
REPLACE,TAPE7=STSTDAT.
EXIT,U.
REPLACE,OUTPUT=PUTOUT1.
EXIT,U.
COST,LO=F.
EXIT,U.
DAYFILE,DFXSTST.
REPLACE,DFXSTST.
```

5. File VD794 is the file that contains measured values. An example of this file is given in Figure B1. The first 40 characters of the first line are for informational purposes; the rest of the file contains measured data. All of the data for a particular variable should

```
EAU GALLE 1980 MEASURED DATA STA. 20
 20   1 800104  11    8.8       4.000  8.0       3.900  7.0       3.500  6.0       3.500
                      5.0       3.400  4.0       3.500  3.0       3.500  2.0       3.200
                      1.0       2.300  0.5       0.800  0.0       0.000
 20   1 800117  11    9.0       4.900  8.0       3.900  7.0       3.300  6.0       3.300
                      5.0       3.400  4.0       3.400  3.0       3.300  2.0 [illegible]
                      1.5       2.900  1.0       0.900  0.0       0.100
 20   1 800130  11    9.0       4.500  8.0       4.000  7.0       4.000  6.0       4.000
                      5.0       4.000  4.0       3.800  3.0       3.500  2.0       3.000
                      1.5       1.400  1.0       0.900  0.0       0.200
 20   1 800214  10    9.0       5.000  8.0       3.900  7.0       3.700  6.0       3.700
                      5.0       3.800  4.0       3.800  3.0       3.300  2.0       1.800
                      1.0       0.500  0.0       0.100
 20   8 800130   5    8.0      53.800  6.0      53.711  4.0      58.244  2.0      37.089
                      0.0      45.867
 20   8 800214   5    8.0      63.289  6.0      14.556  4.0      26.444  2.0      14.356
                      0.0      29.089
 20   8 800228   5    8.0      69.400  6.0      13.333  4.0      14.778  2.0      13.844
                      0.0       9.444
 20   8 800313   5    8.0      10.578  6.0       9.133  4.0      10.444  2.0       9.956
                      0.0      11.422
 20   8 800422   5    8.0      11.133  6.0      14.556  4.0      14.756  2.0      10.467
                      0.0      14.311
 20   8 800429   7    8.0      10.156  6.0       9.933  4.0      10.667  3.0       9.400
                      2.0      10.933  1.0      11.289  0.0      15.178
 20   8 800507   9    8.0      12.333  7.0      11.689  6.0      12.489  5.0 [illegible]
                      4.0      10.400  3.0       9.356  2.0      12.667  1.0       8.644
                      0.0      14.667
```

Figure B1. An example of the data set File VD794 which contains measured values used by the statistical package

be grouped together; within each group, data should be ordered according to date. For each date the following information is needed. The first line contains three variables describing a block of data. Columns 5 and 6 contain a code number for each variable. (A list of the variables and their code numbers are given in Table B1.) Columns 8 through 13 contain the date on which the block of data was measured: columns 8 and 9 contain the last digits of the year, columns 10 and 11 contain the numerical description of the month, and columns 12 and 13 contain the day of the month. Columns 15 through 17 contain the number of data points for that block of data. Each data point consists of a pair of numbers: the first is the depth, in meters, where the sample was measured; the second number is the concentration of the variable. The depth is measured from the surface, and the data are ordered from the bottom to the surface. There are four pairs of numbers on each line in columns 19-22 and 24-32, 34-37 and 39-47, 49-52 and 54-62, and 64-67 and 69-77.

6. File GRADAT is the file that was created in the previous execution. File STSWICH is a one-line file containing information on variables for which statistics will be performed. A '1' in a particular

Table B1

Variables and Their Codes for the Statistical Package

Code	Variable
1	Temperature
2	Zooplankton
3	Algae 1
4	Algae 2
6	Total manganese
7	Detritus
8	Dissolved organic matter
9	Ortho-Phosphate - P
10	Inorganic carbon
11	Ammonia - N
12	Nitrite - N
13	Nitrate - N
14	Oxygen
15	Carbon dioxide
16	pH
17	Alkalinity
18	Total dissolved solids
19	Suspended solids
20	Total iron
21	Sulfate
22	Reduced manganese
23	Reduced iron
24	Iron sulfide
25	Reduced sulfide
26	Coliforms

column will cause the statistical analysis to be performed. The column code for variables is presented in Table B1.

7. Upon successful completion of the execution, four files will be created and permanently stored. File MAPSTST contains the storage location map. File STSTDAT contains statistical output of which an example is given in Figure B2. File PUTOUT1 contains information concerning problems during execution. File DFXSTST is the dayfile which describes the execution.

8. A listing of the statistical package is presented in Figure B3.

```
                              STATISTICAL PROGRAM FOR CE-QUAL-R1 COMPARING FILES
            DEGRAY79 ST.4                                AND  DEGRAY 79 PLNT MAY 6 82 J.W.


      RELIABILITY INDEX  LEGGETT AND WILLIAMS ECOLOGICAL MODELLING 13(1981)303-312
      PAIRED T TEST FOR MEANS SOKAL AND ROHLF 1969 BIOMETRY W.H.FREEMAN AND COMPANY
      NORMALIZED MEAN ERROR (SUM(ABS(P-O)/O)*100.)/N
      COEFFICIENTS FOR THE LINEAR REGRESSION EQUATION


  VARIABLE     DATE     NUMBER OF    OBSERVED     PREDICTED       T       RELIABILITY  NORMALIZED
              YYMMDD   COMPARISONS     MEAN          MEAN      STATISTIC     INDEX     MEAN ERROR
 TEMP         790206       47        .430E+01     .412E+01     .579E+01    .107E+01    .408E+01
 TEMP         790220       47        .433E+01     .413E+01     .116E+02    .105E+01    .441E+01
 TEMP         790306       49        .539E+01     .562E+01    -.290E+01    .112E+01    .961E+01
 TEMP         790320       47        .660E+01     .677E+01    -.144E+01    .113E+01    .112E+02
 TEMP         790403       49        .759E+01     .771E+01    -.846E+00    .115E+01    .123E+02

 TEMP      ALL DATES      239        .566E+01     .569E+01    -.774E+00    .111E+01    .837E+01
 A=-.383E+00  B= .107E+01  T FOR SLOPES= .364E+01  T FOR INTERCEPTS=,-.316E+01  R SQUARE= .923E+00  ST.ERROR OF EST.= .980E+01

  VARIABLE     DATE     NUMBER OF    OBSERVED     PREDICTED       T       RELIABILITY  NORMALIZED
              YYMMDD   COMPARISONS     MEAN          MEAN      STATISTIC     INDEX     MEAN ERROR
 OXYGEN       790206       36        .111E+02     .115E+02    -.143E+02    .104E+01    .366E+01
 OXYGEN       790220       35        .112E+02     .133E+02    -.298E+02    .119E+01    .187E+02
 OXYGEN       790306       49        .118E+02     .147E+02    -.218E+02    .125E+01    .240E+02
 OXYGEN       790320       35        .113E+02     .153E+02    -.825E+01    .140E+01    .365E+02
 OXYGEN       790403       36        .107E+02     .145E+02    -.796E+01    .139E+01    .354E+02

 OXYGEN    ALL DATES      191        .113E+02     .139E+02    -.166E+02    .128E+01    .236E+02
 A= .725E+00  B= .117E+01  T FOR SLOPES= .443E+00  T FOR INTERCEPTS=, .168E+00  R SQUARE= .469E-01  ST.ERROR OF EST.= .302E+02
```

Figure B2. An example of output from the statistical package

```
      PROGRAM  STSTIC(TAPE22,TAPE23,TAPE6,TAPE7)
*
*    STATISTICAL PROGRAM FOR CE-QUAL-R1 COMPARING MEASURED
*    AND PREDICTED VALUES
*
      DIMENSION  ITITLE(2,4),KODEO(450),KDATO(450),KPTO(450),
     *     DEPO(450,50),VALUO(450,50),NAMES(26),NSWICH(50),VALU(70),
     *   VALUP(70),DEPP(70)
      DATA NAMES/'TEMP','ZOOPLANK','ALGAE1','ALGAE2','ALGAE3',
     *   'MN2+MN4','DETRITUS','D.O.M.','PO4-P','T.I.C.','NH4-N',
     *   'NO2-N','NO3-N','OXYGEN','CO2','PH','ALKLINITY','T.D.S.',
     *   'S.S.1','T.IRON','SULFATE','R.MN','R.FE','FE-S','SULFIDE',
     *   'COLIFORM'/
      DATA  KODOLD/1/,NSTOP/0/
      READ(22,30)(ITITLE(1,I),I=1,4)
      READ(23,30)(ITITLE(2,I),I=1,4)
       WRITE(7,29)(ITITLE(1,I),I=1,4),(ITITLE(2,I),I=1,4)
   29 FORMAT(1H1,40X,
     *50HSTATISTICAL PROGRAM FOR CE-QUAL-R1 COMPARING FILES,
     * /,20X,4A10,3X,3HAND,3X,4A10,///)
       WRITE(7,27)
   27 FORMAT(9X,39HRELIABILITY INDEX  LEGGETT AND WILLIAMS
     * ,37H ECOLOGICAL MODELLING 13(1981)303-312,/,
     *9X,53HPAIRED T TEST FOR MEANS SOKAL AND ROHLF 1969 BIOMETRY,
     *24H W.H.FREEMAN AND COMPANY,/,
     *9X,21HNORMALIZED MEAN ERROR,
     *25H (SUM(ABS(P-O)/O)*100.)/N,
     */,9X,47HCOEFFICIENTS FOR THE LINEAR REGRESSION EQUATION,///)
         READ(6,28)(NSWICH(J),J=1,50)
   28    FORMAT(50I1)
   30 FORMAT(4A10)
      I=0
   32 I=I+1
      READ(22,35)KODEO(I),KDATO(I),KPTO(I),KT,
     * (DEPO(I,K),VALUO(I,K),K=1,KT)
      IF(EOF(22).NE.0)GO TO 34
      IF(KT.EQ.4)BACKSPACE 22
      GO TO 32
   34 II=I-1
   35 FORMAT(4X,I2,1X,I6,1X,I3,T15,I3,1X,4(F4.1,1X,F9.3,1X),/,
     *  (18X,F4.1,1X,F9.3,1X,F4.1,1X,F9.3,1X,F4.1,1X,F9.3,1X,
     * F4.1,1X,F9.3))
   40 READ(23,35)KODEP,KDATP,KPTP,KT,(DEPP(I),VALUP(I),I=1,KT)
      IF(EOF(23).NE.0)GO TO 198
      IF(KT.EQ.4)BACKSPACE 23
      IF(KODOLD.NE.KODEP)GO TO 200
   44 IF(NSWICH(KODEP).NE.0)GO TO 46
      KODOLD=KODEP
      GO TO 40
   46 DO 55 I=1,II
         JJ=I
         IF(KODEP.NE.KODEO(I).OR.KDATP.NE.KDATO(I))GO TO 55
         GO TO 74
   55 CONTINUE
       GO TO 40
   74 J=0
*
*    FIGURE WHICH LAYER PREDICTIONS WILL BE USED
*
      KT=KPTO(JJ)
```

Figure B3. A listing of the statistical package
(Sheet 1 of 4)

```
      DO 80 I=1,KT
 76      J=J+1
         IF(DEPP(J).GT.DEPO(JJ,I))GO TO 76
         DI=ABS(DEPP(J)-DEPO(JJ,I))
         IF(ABS(DEPP(J-1)-DEPO(JJ,I)).LT.DI)J=J-1
         VALU(I)=VALUP(J)
         J=J-1
 80   CONTINUE
*
*   T STATISTIC FOR MEANS
*
      RDAL2=0.
       RDAL=0.
      OB=0
      PR=0
      DO 82 I=1,KT
         RDAL2=RDAL2+(VALUO(JJ,I)-VALU(I))**2.
         RDAL=RDAL+VALUO(JJ,I)-VALU(I)
         OB=OB+VALUO(JJ,I)
 82      PR=PR+VALU(I)
      OBT=OBT+OB
      PRT=PRT+PR
      OBA=OB/KT
      PRA=PR/KT
      KTTOT=KTTOT+KT
       RS2T=RS2T+RDAL2
      RST=RST+RDAL
      ZT=KT
       ZRT=(OBA-PRA)/SQRT(((ZT*RDAL2)-RDAL**2.)/(ZT**2.*(ZT-1.)))
      S=0
      SK=0
*
*   RELIABILITY INDEX
*
      DO 90 I=1,KT
         IF(VALU(I).EQ.0)GO TO 90
         SK=SK+1.
         R=VALUO(JJ,I)/VALU(I)
         S=((1.-R)/(1.+R))**2+S
 90   CONTINUE
      STOT=STOT+S
      SKTOT=SKTOT+SK
         IF(SK.EQ.0)GO TO 96
      AB=1.+(SQRT((1./SK)*S))
      AC=1.-(SQRT((1./SK)*S))
      AK=AB/AC
*
*   NORMALIZED MEAN ERROR
*
 96   P=0
      SL=0
      DO 110 I=1,KT
         IF(VALUO(JJ,I).EQ.0)GO TO 110
         SL=SL+1.
         P=(ABS(VALU(I)-VALUO(JJ,I))/VALUO(JJ,I))+P
110   CONTINUE
      PTOT=PTOT+P
      SLTOT=SLTOT+SL
         IF(SL.EQ.0)GO TO 111
      F=(P*100.)/SL
```

Figure B3. (Sheet 2 of 4)

```
*
*   COEFFICIENTS FOR THE LINEAR EQUATION
*   CALCULATED ONLY OVER ALL TIMES
*
      DO 300 I=1,KT
      SUMA=SUMA+VALUO(JJ,I)
      SUMA2=SUMA2+VALUO(JJ,I)**2.
      SUMP=SUMP+VALU(I)
      SUMP2=SUMP2+VALU(I)**2.
      SUMAP=SUMAP+VALUO(JJ,I)*VALU(I)
  300 CONTINUE
      SUMKT=SUMKT+KT
      IF(NSWCH2.EQ.0)WRITE(7,114)
      NSWCH2=1
  114 FORMAT(1H0,2X,8HVARIABLE,5X,4HDATE,5X,9HNUMBER OF,4X,8HOBSERVED,
     * 5X,9HPREDICTED,7X,1HT,7X,11HRELIABILITY,3X,10HNORMALIZED,/,14X,
     * 6HYYMMDD,3X,11HCOMPARISONS,5X,4HMEAN,10X,4HMEAN,6X,9HSTATISTIC
     * ,5X,5HINDEX,7X,10HMEAN ERROR)
  111 WRITE(7,112)NAMES(KODEP),KDATP,KT,OBA,PRA,ZRT,AK,F
  112 FORMAT(1X,A10,3X,I6,6X,I4,6X,5(E10.3,3X))
*
*   CALCULATE STATISTICS FOR A PARTICULAR VARIABLE
*   OVER ALL TIMES AND DEPTHS
*
      GO TO 40
  198 NSTOP=1
  200 CONTINUE
      IF(NSWICH(KODOLD).NE.1)GO TO 214
      A=OBT/KTTOT
      B=PRT/KTTOT
      AB=1.+(SQRT((1./SKTOT)*STOT))
      AC=1.-(SQRT((1./SKTOT)*STOT))
      AK=AB/AC
      F=(PTOT*100.)/SLTOT
      ZRT=(A-B)/SQRT(((SKTOT*RS2T)-RST**2.)/
     * (SKTOT**2.*(SKTOT-1.)))
      AVEA=SUMA/SUMKT
      AVEP=SUMP/SUMKT
      FA=(SUMA2-SUMA**2./SUMKT)/(SUMKT-1.)
      FP=(SUMP2-SUMP**2./SUMKT)/(SUMKT-1.)
      FAP=(SUMAP-SUMA*SUMP/SUMKT)/(SUMKT-1.)
      ESTB=FAP/FA
      ESTA=AVEP-ESTB*AVEA
      SD=(SUMKT-1.)*ESTB**2.*FA
      ST=(SUMKT-1.)*FP
      SI=(ST-SD)/(SUMKT-2.)
      VB=SI/((SUMKT-1.)*FA)
      VA=SI*((SUMKT-1.)*FA+SUMKT*AVEA**2.)/
     * (SUMKT*(SUMKT-1.)*FA)
      TSLOPE=(ESTB-1.)/SQRT(VB)
      TNTCPT=ESTA/SQRT(VA)
      RSQ=SD/ST
      STDRD2=(SUMP2-SUMP**2./SUMKT)-ESTB**2.*(SUMA2-SUMA**2./SUMKT)
      STDRD=SQRT(STDRD2)
      WRITE(7,121)NAMES(KODOLD),KTTOT,A,B,ZRT,AK,F
  121 FORMAT(1H0,A10,10H ALL DATES,5X,I4,6X,5(E10.3,3X))
      WRITE(7,301)ESTA,ESTB,TSLOPE,TNTCPT,RSQ,STDRD
  301 FORMAT(1X,2HA=,E9.3,2X,2HB=,E9.3,15H  T FOR SLOPES=,E9.3,
     * 20H  T FOR INTERCEPTS=,E9.3,11H  R SQUARE=,E9.3,
     * 19H  ST.ERROR OF EST.=,E9.3)
```

Figure B3. (Sheet 3 of 4)

```
      IF(NSTOP.EQ.1)GO TO 500
      NSWCH2=0
      ORT=0.
      PRT=0.
      KTTOT=0.
      SKTOT=0.
      STOT=0.
      SLTOT=0.
      RS2T=0.
      RST=0.
      PTOT=0.
       SUMA=0.
       SUMA2=0.
       SUMP=0.
       SUMP2=0.
       SUMAP=0.
       SUMKT=0.
  214 KODOLD=KODEP
      GO TO 14
  500 STOP
      END
```

Figure B3. (Sheet 4 of 4)

APPENDIX C: FLUX PACKAGE

1. As with CE-QUAL-R1, the flux package resides on the Boeing Mainstream-EKS interactive time-sharing computer system. A user must have his own account number and should have some knowledge of Boeing procedures. To execute the flux package, prepare a file as follows for use by the SUBMIT directive:

```
FLXXEQ,CM300000,T300,P01.
USER,ID,PASWORD.
GET,FLXOBJ/UN=CEROB5.
GET,TAPE61=PLDGFLX.
GET,TAPE5=FLXDDAY.
FILE,TAPE6,FF=YES.
LOADXEQ,F=FLXOBJ,M=FULL/MAP2.
EXIT,U.
REPLACE,MAP2.
REPLACE,TAPE6=OUTPF.
REPLACE,OUTPUT=PUTOUT1.
EXIT,U.
COST,LO=F.
EXIT,U.
DAYFILE,DAYFX.
REPLACE,DAYFX.
```

2. Names that are underlined can be changed at the user's discretion. File PLDGFLX is the file on which information from a CE-QUAL-R1 simulation is stored. File FLXDDAY (see Figure C1) is a four-line file containing information needed for output. The first line contains the hour of the year for which output is requested; up to 16 values can be specified in fields of five characters each. The second line contains either a blank or a '1' in the first 16 columns. A '1' signifies that information is needed for a particular variable; the 16 variables for which information is gathered are listed in Table C1.

```
                1    1    2
Column  1   5   0    5    0

       1032 1056 1296 1536
       111 111111
       SURFACE   CUBICM
           1  168   24
```

Figure C1. An example of file FLXDDAY

Table C1

Variables for Which Flux Information is Available

Column	Variable
1	Fish 1
2	Fish 2
3	Fish 3
4	Benthos
5	Zooplankton
6	Algae 1
7	Algae 2
8	Detritus
9	Sediment
10	Dissolved Organic Matter
11	Ortho-Phosphate - P
12	Carbon
13	Ammonia - N
14	Nitrite - N
15	Nitrate - N
16	Oxygen

3. The third line of FLXDDAY contains two variables. The first variable concerns how the fluxes are to be summed according to layers. (It must be remembered that CE-QUAL-R1 contains a variable-layer scheme and that the layers are numbered from the bottom to the surface. Throughout the year the number of layers may change, so that the surface layer may not always have the same layer number. If the user is interested in a particular process occurring at the surface--for example, surface aeration--he would have to look at different layer numbers

during different times of the year. To make it easier to study the fluxes occurring in the epilimnion, it is possible to sum fluxes in relation to the surface by putting the word SURFACE in columns 1 through 7 of the third card. Otherwise, the fluxes will be summed from the bottom of the reservoir). The second variable concerns units of output: if the word CUBICM is specified in columns 11 through 16, fluxes will be reported in g/cu m; fluxes will be reported in units of kg/layer with any other specification.

4. The fourth line of FLXDDAY contains three variables, the first of which concerns the number of time steps for which fluxes are to be accumulated; the value is shown in columns 1 through 5, right-justified. For example, if the original simulation used a 24-hour time step, a '1' in column 5 would give information on fluxes on a daily basis; a value of 30 would accumulate fluxes for periods of approximately 1 month. The second variable, in columns 6 through 10, represents hours and allows output to be specified at particular intervals (this information is output in addition to that specified in the first line). The third variable, in columns 11 through 15, specifies the Julian date for the start of the simulation.

5. Upon satisfactory completion of the execution, four files will be created and permanently stored. File MAP2 contains the storage location map. File OUTPF is the normal output from the flux package; an example of output is given in Figure C2. File PUTOUT1 contains information concerning problems during execution. File DAYFX is the dayfile which describes the execution.

DEGRAY 79 ANAER MARCH 19 82 J.W.

FLUX PROGRAM DOES NOT INCLUDE MACROPHYTES OR ANAEROBIC MATERIALS

SIMULATION HOUR= 744 LOWEST NUMBER OF LAYERS= 55 LAYERS NUMBERED FROM THE SURFACE

FLUXES ARE IN KG/LAYER ACCUMULATED OVER THE LAST 7 SIMULATION TIME STEPS

##

##

FLUX FOR THE OXYGEN COMPARTMENT

LAYER	ALGAE PHOTOSYNTHESIS	ALGAE RESPIRATION	DECAY OF AMMONIA	DECAY OF NITRITE	DETRITUS DECOMPOSITION	SEDIMENT DECOMPOSITION	ZOOPLANKTON RESPIRATION	BENTHOS RESPIRATION	FISH RESPIRATION
1	.5711E+04	-.1151E+04	-.6551E+03	-.1536E+02	-.4517E+01	-.2187E+04	-.8033E+02	-.4489E+03	-.2269E+03
2	.8276E+04	-.1815E+04	-.7605E+03	-.1773E+02	-.5762E+01	-.2874E+04	-.1015E+03	-.5701E+03	-.2936E+03
3	.7754E+04	-.1773E+04	-.7387E+03	-.1727E+02	-.5653E+01	-.2858E+04	-.9832E+02	-.5615E+03	-.2856E+03
4	.6267E+04	-.1684E+04	-.7040E+03	-.1647E+02	-.5376E+01	-.2763E+04	-.9355E+02	-.5438E+03	-.2738E+03
5	.4701E+04	-.1592E+04	-.6694E+03	-.1567E+02	-.5088E+01	-.2661E+04	-.8878E+02	-.5255E+03	-.2619E+03
6	.3444E+04	-.1501E+04	-.6341E+03	-.1485E+02	-.4802E+01	-.2556E+04	-.8402E+02	-.5067E+03	-.2500E+03
7	.2323E+04	-.1426E+04	-.5988E+03	-.1400E+02	-.4564E+01	-.2471E+04	-.7948E+02	-.4882E+03	-.2206E+03
8	.1578E+04	-.1347E+04	-.5670E+03	-.1326E+02	-.4312E+01	-.2378E+04	-.7522E+02	-.4709E+03	-.2058E+03
9	.1051E+04	-.1273E+04	-.5366E+03	-.1255E+02	-.4075E+01	-.2293E+04	-.7118E+02	-.4542E+03	-.2161E+03
10	.6910E+03	-.1203E+04	-.5075E+03	-.1186E+02	-.3851E+01	-.2211E+04	-.6732E+02	-.4381E+03	-.2134E+03
11	.3990E+03	-.1136E+04	-.4796E+03	-.1121E+02	-.3637E+01	-.2127E+04	-.6362E+02	-.4224E+03	-.1713E+03
12	0.	-.1072E+04	-.4528E+03	-.1058E+02	-.3432E+01	-.2046E+04	-.6006E+02	-.4070E+03	-.1637E+03
13	0.	-.1011E+04	-.4271E+03	-.9982E+01	-.3236E+01	-.1970E+04	-.5666E+02	-.3920E+03	-.1563E+03
14	0.	-.9528E+03	-.4023E+03	-.9404E+01	-.3049E+01	-.1895E+04	-.5338E+02	-.3773E+03	-.1492E+03
15	0.	-.8965E+03	-.3786E+03	-.8848E+01	-.2868E+01	-.1823E+04	-.5023E+02	-.3629E+03	-.1423E+03
16	0.	-.8435E+03	-.3564E+03	-.8331E+01	-.2699E+01	-.1753E+04	-.4727E+02	-.3491E+03	-.1358E+03
17	0.	-.7873E+03	-.3342E+03	-.7814E+01	-.2523E+01	-.1675E+04	-.4424E+02	-.3343E+03	-.1290E+03
18	0.	-.7417E+03	-.3134E+03	-.7326E+01	-.2373E+01	-.1614E+04	-.4158E+02	-.3215E+03	-.1229E+03
19	0.	-.6927E+03	-.2924E+03	-.6833E+01	-.2216E+01	-.1544E+04	-.3882E+02	-.3074E+03	-.1165E+03
20	0.	-.6483E+03	-.2738E+03	-.6400E+01	-.2074E+01	-.1480E+04	-.3633E+02	-.2948E+03	-.1107E+03
21	0.	-.6054E+03	-.2557E+03	-.5974E+01	-.1937E+01	-.1418E+04	-.3393E+02	-.2823E+03	-.1051E+03
22	0.	-.5636E+03	-.2379E+03	-.5559E+01	-.1803E+01	-.1354E+04	-.3158E+02	-.2696E+03	-.9945E+02
23	0.	-.5240E+03	-.2212E+03	-.5169E+01	-.1676E+01	-.1292E+04	-.2937E+02	-.2574E+03	-.9409E+02
24	0.	-.4850E+03	-.2047E+03	-.4782E+01	-.1551E+01	-.1229E+04	-.2718E+02	-.2448E+03	-.8866E+02
25	0.	-.4488E+03	-.1893E+03	-.4423E+01	-.1435E+01	-.1169E+04	-.2515E+02	-.2329E+03	-.8358E+02
26	0.	-.4145E+03	-.1748E+03	-.4082E+01	-.1325E+01	-.1111E+04	-.2323E+02	-.2213E+03	-.7869E+02
27	0.	-.3824E+03	-.1613E+03	-.3767E+01	-.1223E+01	-.1056E+04	-.2143E+02	-.2102E+03	-.7407E+02
28	0.	-.3512E+03	-.1481E+03	-.3458E+01	-.1123E+01	-.9993E+03	-.1968E+02	-.1990E+03	-.6946E+02
29	0.	-.3241E+03	-.1366E+03	-.3189E+01	-.1036E+01	-.9515E+03	-.1816E+02	-.1895E+03	-.6552E+02
30	0.	-.2960E+03	-.1247E+03	-.2910E+01	-.9460E+00	-.8977E+03	-.1658E+02	-.1788E+03	-.6121E+02
31	0.	-.2697E+03	-.1136E+03	-.2650E+01	-.8619E+00	-.8459E+03	-.1511E+02	-.1685E+03	-.5712E+02
32	0.	-.2449E+03	-.1031E+03	-.2405E+01	-.7826E+00	-.7954E+03	-.1372E+02	-.1584E+03	-.5318E+02
33	0.	-.2208E+03	-.9335E+02	-.2179E+01	-.7067E+00	-.7440E+03	-.1240E+02	-.1485E+03	-.4940E+02

Figure C2. An example of output from the flux package (Sheet 1 of 3)

34	0.	-.2000E+03	-.8413E+02	-.1962E+01	-.6390E+00	-.6994E+03	-.1121E+02	-.1393E+03	-.4583E+02
35	0.	-.1796E+03	-.7546E+02	-.1759E+01	-.5736E+00	-.6530E+03	-.1006E+02	-.1301E+03	-.4235E+02
36	0.	-.1608E+03	-.6751E+02	-.1573E+01	-.5134E+00	-.6089E+03	-.9006E+01	-.1213E+03	-.3908E+02
37	0.	-.1430E+03	-.5999E+02	-.1397E+01	-.4565E+00	-.5651E+03	-.8009E+01	-.1125E+03	-.3588E+02
38	0.	-.1267E+03	-.5310E+02	-.1236E+01	-.4043E+00	-.5234E+03	-.7095E+01	-.1043E+03	-.3289E+02
39	0.	-.1115E+03	-.4665E+02	-.1086E+01	-.3555E+00	-.4826E+03	-.6241E+01	-.9612E+02	-.2999E+02
40	0.	-.9750E+02	-.4074E+02	-.9474E+00	-.3108E+00	-.4433E+03	-.4579E+01	-.8830E+02	-.2724E+02
41	0.	-.8470E+02	-.3533E+02	-.8209E+00	-.2698E+00	-.4056E+03	-.3973E+01	-.8079E+02	-.2465E+02
42	0.	-.7297E+02	-.3038E+02	-.7052E+00	-.2323E+00	-.3692E+03	-.3418E+01	-.7355E+02	-.2219E+02
43	0.	-.6199E+02	-.2589E+02	-.6005E+00	-.1975E+00	-.3328E+03	-.2917E+01	-.6646E+02	-.1983E+02
44	0.	-.5236E+02	-.2179E+02	-.5048E+00	-.1666E+00	-.2993E+03	-.2458E+01	-.5977E+02	-.1762E+02
45	0.	-.4375E+02	-.1814E+02	-.4195E+00	-.1390E+00	-.2675E+03	-.2049E+01	-.5342E+02	-.1556E+02
46	0.	-.3608E+02	-.1489E+02	-.3436E+00	-.1145E+00	-.2373E+03	-.1684E+01	-.4740E+02	-.1363E+02
47	0.	-.2928E+02	-.1201E+02	-.2762E+00	-.9270E-01	-.2086E+03	-.1361E+01	-.4166E+02	-.1183E+02
48	0.	-.2331E+02	-.9485E+01	-.2172E+00	-.7359E-01	-.1814E+03	-.1077E+01	-.3624E+02	-.1015E+02
49	0.	-.1811E+02	-.7285E+01	-.1658E+00	-.5695E-01	-.1557E+03	-.8305E+00	-.3110E+02	-.8591E+01
50	0.	-.1365E+02	-.5400E+01	-.1218E+00	-.4269E-01	-.1317E+03	-.6191E+00	-.2631E+02	-.7157E+01
51	0.	-.9867E+01	-.3795E+01	-.8428E-01	-.3056E-01	-.1092E+03	-.4393E+00	-.2182E+02	-.5840E+01
52	0.	-.6029E+01	-.2009E+01	-.4038E-01	-.1785E-01	-.7520E+02	-.2486E+00	-.1499E+02	-.3922E+01
53	0.	-.3798E+01	-.1181E+01	-.2292E-01	-.1101E-01	-.5550E+02	-.1478E+00	-.1105E+02	-.2841E+01
54	0.	-.2139E+01	-.5986E+00	-.1095E-01	-.6013E-02	-.3744E+02	-.7481E-01	-.7454E+01	-.1880E+01
55	0.	-.1096E+01	-.2478E+00	-.3772E-02	-.2918E-02	-.2252E+02	-.3181E-01	-.4474E+01	-.1103E+01
56	0.	-.4426E+00	-.7889E-01	-.1010E-02	-.1117E-02	-.1073E+02	-.7386E-02	-.2132E+01	-.5123E+00
57	0.	-.1745E+00	-.2378E-01	-.2408E-03	-.4189E-03	-.4441E+01	-.5574E-03	-.8843E+00	-.2076E+00
58	0.	-.7423E-01	-.9419E-02	-.8790E-04	-.1762E-03	-.2157E+01	0.	-.4303E+00	-.1002E+00
59	0.	-.2670E-01	-.3387E-02	-.3161E-04	-.6336E-04	-.1185E+01	0.	-.2364E+00	-.5506E-01
60	0.	-.2080E-02	-.2640E-03	-.2464E-05	-.4938E-05	-.2003E+00	0.	-.3996E-01	-.9304E-02
TOTAL	.4219E+05	-.3016E+05	-.1286E+05	-.3006E+03	-.9722E+02	-.6392E+05	-.1697E+04	-.1271E+05	-.5246E+04

LAYER	DOM DECOMPOSITION	INFLOW	OUTFLOW	SURFACE EXCHANGE	DIFFUSION		NET CONVECTION	OXIDATION	TOTAL
					ABOVE	BELOW			
1	-.6074E+05	.1210E+05	-.4076E+04	.2954E+07	0.	-.1638E+06	-.6647E+06	0.	.2074E+07
2	-.8322E+05	.1127E+05	-.3916E+04	0.	.1638E+06	0.	-.7272E+05	0.	.1703E+05
3	-.8088E+05	.1074E+05	-.3879E+04	0.	0.	0.	-.3546E+04	0.	-.7615E+05
4	-.7691E+05	.1024E+05	-.3845E+04	0.	0.	0.	.1195E+05	0.	-.5839E+05
5	-.7288E+05	.9749E+04	-.3812E+04	0.	0.	0.	.1585E+05	0.	-.5221E+05
6	-.6889E+05	.9265E+04	-.3774E+04	0.	0.	0.	.1727E+05	0.	-.4824E+05
7	-.6528E+05	.3590E+04	-.3712E+04	0.	0.	0.	.3766E+05	0.	-.3072E+05
8	-.6174E+05	.3406E+04	-.3673E+04	0.	0.	0.	.3668E+05	0.	-.2881E+05
9	-.5839E+05	.3228E+04	-.3635E+04	0.	0.	0.	.3538E+05	0.	-.2723E+05
10	-.5521E+05	.3056E+04	-.3596E+04	0.	0.	0.	.3761E+05	0.	-.2210E+05
11	-.5216E+05	.2890E+04	-.3557E+04	0.	0.	0.	.3843E+05	0.	-.1842E+05
12	-.4924E+05	.2729E+04	-.3517E+04	0.	0.	0.	.3685E+05	0.	-.1739E+05
13	-.4644E+05	.2575E+04	-.3478E+04	0.	0.	0.	.3633E+05	0.	-.1504E+05
14	-.4376E+05	.2427E+04	-.3437E+04	0.	0.	0.	.3765E+05	0.	-.1096E+05
15	-.4118E+05	.2284E+04	-.3397E+04	0.	0.	0.	.3468E+05	0.	-.1128E+05
16	-.3874E+05	.2150E+04	-.3357E+04	0.	0.	0.	.3401E+05	0.	-.9439E+04

Figure C2. (Sheet 2 of 3)

17	-.3623E+05	.2017E+04	-.3316E+04	0.	0.	0.	.3087E+05	0.	-.9973E+04
18	-.3407E+05	.1891E+04	-.3274E+04	0.	0.	0.	.2854E+05	0.	-.1008E+05
19	-.3182E+05	.1764E+04	-.3226E+04	0.	0.	0.	.2595E+05	0.	-.1033E+05
20	-.2978E+05	.1652E+04	-.3187E+04	0.	0.	0.	.2360E+05	0.	-.1057E+05
21	-.2781E+05	.1543E+04	-.3147E+04	0.	0.	0.	.2155E+05	0.	-.1058E+05
22	-.2589E+05	.1436E+04	-.3103E+04	0.	0.	0.	.1960E+05	0.	-.1052E+05
23	-.2407E+05	.1335E+04	-.3059E+04	0.	0.	0.	.1777E+05	0.	-.1045E+05
24	-.2228E+05	.1235E+04	-.3010E+04	0.	0.	0.	.1603E+05	0.	-.1031E+05
25	-.2062E+05	.1142E+04	-.2964E+04	0.	0.	0.	.1451E+05	0.	-.1008E+05
26	-.1904E+05	.1055E+04	-.2918E+04	0.	0.	0.	.1339E+05	0.	-.9542E+04
27	-.1756E+05	.9729E+03	-.2873E+04	0.	0.	0.	.1237E+05	0.	-.8999E+04
28	-.1613E+05	.8934E+03	-.2825E+04	0.	0.	0.	.1139E+05	0.	-.8461E+04
29	-.1488E+05	.8243E+03	-.2288E+04	0.	0.	0.	.1054E+05	0.	-.7499E+04
30	-.1359E+05	.7523E+03	-.2247E+04	0.	0.	0.	.9652E+04	0.	-.7016E+04
31	-.1239E+05	.6851E+03	-.2207E+04	0.	0.	0.	.8821E+04	0.	-.6561E+04
32	-.1125E+05	.6218E+03	-.2167E+04	0.	0.	0.	.8036E+04	0.	-.6129E+04
33	-.1016E+05	.5638E+03	-.2130E+04	0.	0.	0.	.7303E+04	0.	-.5695E+04
34	-.9188E+04	.5076E+03	-.2087E+04	0.	0.	0.	.6641E+04	0.	-.5309E+04
35	-.8249E+04	.4553E+03	-.2045E+04	0.	0.	0.	.5987E+04	0.	-.4944E+04
36	-.7385E+04	.4073E+03	-.2005E+04	0.	0.	0.	.5387E+04	0.	-.4603E+04
37	-.6567E+04	.3619E+03	-.1960E+04	0.	0.	0.	.5123E+04	0.	-.3970E+04
38	-.5818E+04	.3204E+03	-.1919E+04	0.	0.	0.	.4232E+04	0.	-.4033E+04
39	-.5119E+04	.2815E+03	-.1874E+04	0.	0.	0.	.3721E+04	0.	-.3765E+04
40	-.4476E+04	.2458E+03	-.1829E+04	0.	0.	0.	.3265E+04	0.	-.3498E+04
41	-.3888E+04	.2132E+03	-.1784E+04	0.	0.	0.	.2909E+04	0.	-.3186E+04
42	-.3349E+04	.1833E+03	-.1738E+04	0.	0.	0.	.2551E+04	0.	-.2925E+04
43	-.2856E+04	.1563E+03	-.1692E+04	0.	0.	0.	.2204E+04	0.	-.2693E+04
44	-.2407E+04	.1316E+03	-.1644E+04	0.	0.	0.	.1893E+04	0.	-.2480E+04
45	-.2011E+04	.1096E+03	-.1596E+04	0.	0.	0.	.1592E+04	0.	-.2306E+04
46	-.1658E+04	.8997E+02	-.1548E+04	0.	0.	0.	.1238E+04	0.	-.2230E+04
47	-.1345E+04	.7257E+02	-.1500E+04	0.	0.	0.	.1012E+04	0.	-.2066E+04
48	-.1070E+04	.5731E+02	-.1453E+04	0.	0.	0.	.8187E+03	0.	-.1910E+04
49	-.8312E+03	.4404E+02	-.1408E+04	0.	0.	0.	.6490E+03	0.	-.1768E+04
50	-.6261E+03	.3267E+02	-.1368E+04	0.	0.	0.	.5017E+03	0.	-.1645E+04
51	-.4518E+03	.2301E+02	-.1341F+04	0.	0.	0.	.3746E+03	0.	-.1547E+04
52	-.2742E+03	.1226E+02	-.1147E+04	0.	0.	0.	.2344E+03	0.	-.1277E+04
53	-.1722E+03	.6043E+01	-.9663E+03	0.	0.	0.	.1625E+03	0.	-.1045E+04
54	-.9664E+02	.3154E+01	-.1040E+04	0.	0.	0.	.9862E+02	0.	-.1084E+04
55	-.4921E+02	.1082E+01	-.1150E+04	0.	0.	0.	.5331E+02	0.	-.1175E+04
56	-.1980E+02	.2405E+00	-.1377E+04	0.	0.	0.	.2294E+02	0.	-.1388E+04
57	-.7789E+01	.1801E-01	-.1030E+03	0.	0.	0.	.9720E+01	0.	-.1068E+03
58	-.3313E+0[illegible]	0.	0.	0.	0.	0.	.4706E+01	0.	-.1378E+01
59	-.1191[illegible]	0.	0.	0.	0.	0.	.2194E+01	0.	-.5046E+00
60	-.928[illegible]	0.	0.	0.	0.	0.	.2975E+00	0.	-.4731E-01
TOTAL	-.1391[illegible]	.1158E+06	-.1432E+06	.2954E+07	.1638E+06	-.1638E+06	-.3362E-05	0.	.1451E+07

Figure C2. (Sheet 3 of 3)

DAT

FILM